

n,n-bis(2-cyanoethyl)aspartic acid
6328-90-1 | DTXSID20286167

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.07

Global applicability domain: Inside

Local applicability domain index: 4.57e-01

Confidence level: 4.19e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Oxo-6,7,8,9-tetrahydro-4H-pyrido[1,2-a]pyrimidine-3-carboxamide

Measured: -0.380

Predicted: -0.148

[Image not found](#)

N-Acetyl-L-alanyl-L-alaninamide

Measured: -2.00

Predicted: -1.69